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Di-μ-chlorido-bis{[(1*H*-benzo[*d*]-imidazol-2-ylmethyl)dibenzylamine]-chloridocadmium(II)} ethanol disolvate

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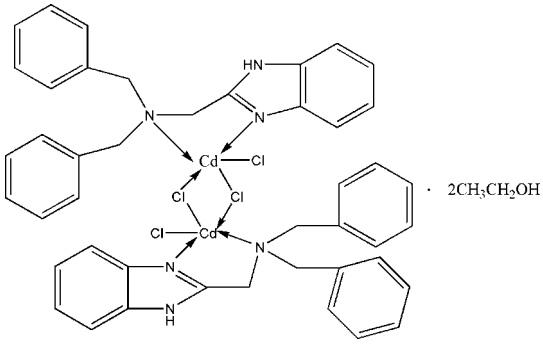
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.004 Å; R factor = 0.027; wR factor = 0.078; data-to-parameter ratio = 20.8.

The title compound, $[Cd_2Cl_4(C_{22}H_{21}N_3)_2]\cdot 2C_2H_6O$, is a centrosymmetric dimer. The Cd^{II} cation shows a distorted tetragonal–pyramidal coordination geometry formed by three Cl^- anions and two N atoms. The $Cd-Cl_{terminal}$ bond distance of 2.4591 (7) Å is much shorter than the $Cd-Cl_{bridging}$ bond distances of 2.5604 (6) and 2.6132 (6) Å. The ethanol solvent molecule is hydrogen bonded with the dimeric complex *via* O—H···Cl hydrogen bonds.

Related literature

The Cd—N1 and Cd—N2 bond distances of 2.4636 (16) and 2.2819 (16) Å are shorter than those found in the literature (Choi & Jeon, 2003; Huang *et al.*, 1998).



Experimental

Crystal data

$[Cd_2Cl_4(C_{22}H_{21}N_3)_2]\cdot 2C_2H_6O$
M_r = 1113.58
Monoclinic, $P2_1/n$
a = 12.6360 (9) Å
b = 13.3620 (10) Å
c = 15.0200 (11) Å
β = 101.955 (5)°
V = 2481.0 (3) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 1.12 mm^{-1}
T = 293 (2) K
0.44 × 0.32 × 0.19 mm

Data collection

Bruker APEX CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.659, T_{max} = 0.812
15017 measured reflections
5827 independent reflections
5067 reflections with $I > 2\sigma(I)$
R_{int} = 0.022

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.027
$wR(F^2)$ = 0.078
S = 1.05
5827 reflections
280 parameters
1 restraint
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.33 e Å^{-3}
$\Delta\rho_{min}$ = −0.69 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Cd1—Cl1	2.4591 (7)	Cd1—N1	2.4636 (16)
Cd1—Cl2	2.5604 (6)	Cd1—N2	2.2819 (16)
Cd1—Cl2^{i}	2.6132 (6)		
N2—Cd1—Cl1	105.92 (5)	N1—Cd1—Cl2	150.72 (5)
N2—Cd1—N1	73.73 (6)	N2—Cd1—Cl2^{i}	148.17 (5)
Cl1—Cd1—N1	99.07 (4)	Cl1—Cd1—Cl2^{i}	102.95 (2)
N2—Cd1—Cl2	96.56 (4)	N1—Cd1—Cl2^{i}	88.84 (4)
Cl1—Cd1—Cl2	110.19 (2)	Cl2—Cd1—Cl2^{i}	85.712 (19)

Symmetry code: (i) $-x+1, -y, -z$.

Table 2
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
O1—H1A···Cl1^{ii}	0.85	2.33	3.157 (2)	164
N3—H3N···O1	0.88	1.90	2.772 (3)	174

Symmetry code: (ii) $x+\frac{1}{2}, -y+\frac{1}{2}, z+\frac{1}{2}$.

Data collection: *SMART* (Bruker, 1997); cell refinement: *SAINT* (Bruker, 1999); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL-Plus* (Sheldrick, 1990); software used to prepare material for publication: *SHELXL97*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: XU2261).

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supplementary materials

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Di-μ-chlorido-bis{[(1*H*-benzo[*d*]imidazol-2-ylmethyl)dibenzylamine]chloridocadmium(II)} ethanol disolvate

G.-J. Ping, J.-F. Ma and L.-P. Zhang

Comment

As part of an investigation of the coordination chemistry of cadmium compounds, we present here the preparation and crystal structure of the title compound.

The title compound is composed of Cd^{II} cations, Cl^{-} anions, 1*H*-benzo[*d*]imidazol-2-yl)-*N*,*N*-dibenzylmethanamine (*L*) and solvent ethanol molecules. It is a centrosymmetric dimer (Fig. 1). Two Cd^{II} cations are bridged by two Cl^{-} anions to form a binuclear compound. Each Cd cation shows a distorted tetragonal pyramid geometry formed by three Cl^{-} anions and two N atoms of *L*. The Cd—N1 and Cd—N2 bond distances (Table 1) are shorter than the values in the literature (Choi & Jeon, 2003; Huang *et al.*, 1998). The Cd—N2 bond distance is much shorter than the Cd—N1 bond distance, indicating comparatively strong coordination. There are hydrogen-bonding interactions in the crystal (Table 2), forming a two-dimensional supramolecular structure (Fig. 2). In addition, solvent ethanol molecules participate in hydrogen-bonding interactions.

Experimental

A mixture of *N*,*N*-dibenzylglycine (10.2 g, 40 mmol) and *o*-phenylenediamine (4.32 g, 40 mmol) in 70 ml e thanediol was reflux for 16 h. The mixture was cooled to room temperature and added in hot water. The mixture was constantly stirred until brown solid was obtained and then filtered. The solid was purified by recrystallized from ethanol-water solution to get ligand *L*. The *L* (0.0654 g, 0.2 mmol) dissolved in hot ethanol (10 ml) was added to a hot ethanol solution (5 ml) of cadmium chloride (0.0457 g, 0.2 mmol). The mixture was stirred at room temperature for 30 min in air and filtered. Crystals suitable for X-ray diffraction were obtained by slow evaporation of the ethanol solution; yield 78%.

Refinement

All H-atoms bound to carbon were refined using a riding model with C—H = 0.93–0.97 Å, U_{iso}(H) = 1.2U_{eq}(C) for aromatic and CH_2, U_{iso}(H) = 1.5U_{eq}(C) for CH_3. The imino and hydroxy H atoms were located in a difference Fourier map and refined in riding mode with U_{iso}(H) = 1.5U_{eq}(O,*N*). The C23—C24 bond distance restraint was used in the refinement for the lattice solvent molecule.

Figures

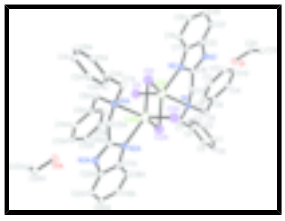


Fig. 1. The molecular structure of the title compound with atom labels and 30% probability displacement ellipsoids for non-H atoms [symmetry codes: (i) 1 − *x*, −*y*, −*z*.]

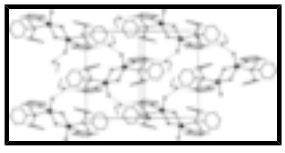


Fig. 2. Two-dimensional supra-molecular layers of the title compound formed by hydrogen bonding (dashed lines) [symmetry codes: (i) 1 − *x*, −*y*, −*z*; (ii) 1/2 + *x*, 0.5 − *y*, 1/2 + *z*].

Di-μ-chlorido-bis{[(1*H*-benzo[*d*]imidazol-2- ylmethyl)dibenzylamine]chloridocadmium(II)} ethanol disolvate

Crystal data

$[Cd_2Cl_4(C_{22}H_{21}N_3)_2]\cdot 2C_2H_6O$	F_{000} = 1128
M_r = 1113.58	D_x = 1.491 Mg m^{-3}
Monoclinic, $P2_1/n$	Mo $K\alpha$ radiation λ = 0.71069 Å
Hall symbol: -P 2yn	Cell parameters from 5067 reflections
a = 12.6360 (9) Å	θ = 1.9–28.3º
b = 13.3620 (10) Å	μ = 1.12 mm^{-1}
c = 15.0200 (11) Å	T = 293 (2) K
β = 101.955 (5)º	Block, colorless
V = 2481.0 (3) Å^3	0.44 × 0.32 × 0.19 mm
Z = 2	

Data collection

Bruker APEX CCD area-detector diffractometer	5827 independent reflections
Radiation source: fine-focus sealed tube	5067 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.022
T = 293(2) K	θ_{max} = 28.3º
ω scans	θ_{min} = 1.9º
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	h = −16→16
T_{min} = 0.659, T_{max} = 0.812	k = −16→15
15017 measured reflections	l = −16→20

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites

$R[F^2 > 2\sigma(F^2)] = 0.027$

$wR(F^2) = 0.078$

$S = 1.05$

5827 reflections

280 parameters

1 restraint

Primary atom site location: structure-invariant direct methods

H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0459P)^2 + 0.1798P]$ where $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{max} < 0.001$

$\Delta\rho_{max} = 0.33$ e Å^{-3}

$\Delta\rho_{min} = -0.69$ e Å^{-3}

Extinction correction: none

Special details

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s involving l.s. planes.

Refinement. Refinement of F^2 against ALL reflections. The weighted *R*-factor *wR* and goodness of fit *S* are based on F^2, conventional *R*-factors *R* are based on *F*, with *F* set to zero for negative F^2. The threshold expression of $F^2 > \sigma(F^2)$ is used only for calculating *R*-factors(gt) *etc*. and is not relevant to the choice of reflections for refinement. *R*-factors based on F^2 are statistically about twice as large as those based on *F*, and *R*- factors based on ALL data will be even larger.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}
Cd1	0.600334 (11)	0.089731 (12)	0.069920 (10)	0.04431 (7)
C1	1.1986 (2)	0.0283 (2)	0.18405 (19)	0.0673 (7)
H1	1.2728	0.0230	0.2064	0.081*
C2	1.1488 (2)	0.1193 (2)	0.1788 (2)	0.0721 (8)
H2	1.1894	0.1764	0.1974	0.087*
C3	1.03876 (19)	0.1275 (2)	0.14614 (18)	0.0599 (6)
H3	1.0061	0.1902	0.1427	0.072*
C4	0.97679 (17)	0.04404 (18)	0.11860 (14)	0.0475 (5)
C5	1.02856 (19)	−0.0472 (2)	0.12327 (19)	0.0630 (6)
H5	0.9886	−0.1045	0.1039	0.076*
C6	1.1384 (2)	−0.0549 (2)	0.1562 (2)	0.0698 (7)
H6	1.1717	−0.1173	0.1594	0.084*
C7	0.85601 (17)	0.0526 (2)	0.08080 (15)	0.0509 (5)
H7A	0.8422	0.1162	0.0494	0.061*
H7B	0.8350	0.0002	0.0360	0.061*
C8	0.79287 (19)	−0.05625 (19)	0.19035 (17)	0.0544 (5)
H8A	0.8630	−0.0635	0.2308	0.065*
H8B	0.7883	−0.1055	0.1423	0.065*
C9	0.70633 (19)	−0.07780 (16)	0.24284 (16)	0.0506 (5)
C10	0.6041 (2)	−0.10782 (18)	0.19770 (18)	0.0554 (6)
H10	0.5914	−0.1204	0.1355	0.067*
C11	0.7238 (2)	−0.0669 (2)	0.33619 (17)	0.0626 (7)
H11	0.7929	−0.0511	0.3685	0.075*

C12	0.6411 (3)	−0.0787 (2)	0.3826 (2)	0.0705 (8)
H12	0.6544	−0.0705	0.4454	0.085*
C13	0.5391 (3)	−0.1027 (2)	0.3355 (2)	0.0679 (7)
H13	0.4824	−0.1077	0.3660	0.082*
C14	0.5207 (2)	−0.1194 (2)	0.24375 (19)	0.0631 (6)
H14	0.4523	−0.1384	0.2124	0.076*
C15	0.81300 (16)	0.12627 (18)	0.21745 (14)	0.0476 (5)
H15A	0.8329	0.1862	0.1883	0.057*
H15B	0.8747	0.1059	0.2638	0.057*
C16	0.71965 (16)	0.14870 (15)	0.26078 (13)	0.0423 (4)
C17	0.55683 (16)	0.16587 (15)	0.28049 (14)	0.0421 (4)
C18	0.44502 (17)	0.16698 (18)	0.27295 (16)	0.0511 (5)
H18	0.3979	0.1579	0.2171	0.061*
C19	0.4073 (2)	0.1820 (2)	0.35138 (17)	0.0596 (6)
H19	0.3331	0.1810	0.3487	0.072*
C20	0.4769 (2)	0.1985 (2)	0.43447 (17)	0.0620 (6)
H20	0.4479	0.2095	0.4857	0.074*
C21	0.5875 (2)	0.19919 (19)	0.44337 (15)	0.0570 (6)
H21	0.6339	0.2105	0.4992	0.068*
C22	0.62618 (17)	0.18215 (16)	0.36486 (14)	0.0452 (4)
C23	0.8661 (7)	0.0467 (6)	0.5860 (4)	0.222 (4)
H23A	0.8736	0.0380	0.6504	0.332*
H23B	0.8922	−0.0120	0.5605	0.332*
H23C	0.7912	0.0568	0.5585	0.332*
C24	0.9298 (5)	0.1349 (5)	0.5682 (3)	0.154 (2)
H24A	0.9035	0.1939	0.5944	0.184*
H24B	1.0049	0.1253	0.5978	0.184*
O1	0.92314 (17)	0.15108 (19)	0.47359 (14)	0.0912 (7)
H1A	0.9779	0.1834	0.4641	0.137*
Cl1	0.64262 (5)	0.23322 (5)	−0.01913 (5)	0.06842 (17)
Cl2	0.39562 (4)	0.06129 (5)	0.03986 (4)	0.05318 (14)
N1	0.78525 (13)	0.04571 (14)	0.14913 (11)	0.0424 (4)
N2	0.61827 (13)	0.14620 (13)	0.21566 (11)	0.0422 (4)
N3	0.72942 (14)	0.17274 (14)	0.34891 (11)	0.0460 (4)
H3N	0.7914	0.1705	0.3880	0.069*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cd1	0.03532 (10)	0.05476 (12)	0.03982 (10)	−0.00554 (6)	0.00081 (6)	−0.00510 (6)
C1	0.0374 (12)	0.0806 (19)	0.0830 (18)	−0.0039 (11)	0.0106 (11)	0.0061 (14)
C2	0.0450 (13)	0.0689 (17)	0.100 (2)	−0.0172 (12)	0.0087 (14)	−0.0007 (15)
C3	0.0477 (12)	0.0529 (13)	0.0789 (17)	−0.0052 (10)	0.0130 (12)	0.0062 (12)
C4	0.0373 (10)	0.0605 (13)	0.0457 (11)	−0.0042 (9)	0.0112 (8)	−0.0043 (10)
C5	0.0441 (12)	0.0613 (15)	0.0863 (18)	−0.0067 (11)	0.0197 (12)	−0.0190 (13)
C6	0.0483 (14)	0.0669 (16)	0.098 (2)	0.0063 (12)	0.0239 (14)	−0.0003 (15)
C7	0.0378 (11)	0.0697 (14)	0.0448 (11)	−0.0048 (10)	0.0081 (9)	−0.0045 (10)
C8	0.0426 (11)	0.0557 (13)	0.0641 (14)	0.0015 (10)	0.0093 (10)	0.0037 (11)

C9	0.0491 (12)	0.0462 (12)	0.0548 (13)	0.0023 (9)	0.0068 (10)	0.0096 (9)
C10	0.0546 (14)	0.0567 (14)	0.0516 (13)	−0.0081 (10)	0.0033 (10)	0.0082 (10)
C11	0.0643 (16)	0.0635 (15)	0.0542 (14)	−0.0095 (12)	−0.0010 (12)	0.0146 (11)
C12	0.089 (2)	0.0696 (18)	0.0518 (14)	−0.0160 (14)	0.0119 (14)	0.0115 (12)
C13	0.0743 (18)	0.0622 (16)	0.0733 (18)	−0.0058 (12)	0.0292 (15)	0.0162 (13)
C14	0.0540 (14)	0.0633 (15)	0.0700 (16)	−0.0092 (12)	0.0084 (12)	0.0173 (13)
C15	0.0356 (10)	0.0579 (12)	0.0464 (11)	−0.0085 (9)	0.0016 (8)	−0.0071 (10)
C16	0.0376 (10)	0.0461 (11)	0.0411 (10)	−0.0067 (8)	0.0033 (8)	−0.0038 (8)
C17	0.0416 (10)	0.0417 (10)	0.0432 (10)	−0.0036 (8)	0.0091 (8)	−0.0013 (8)
C18	0.0422 (11)	0.0564 (13)	0.0547 (12)	−0.0059 (9)	0.0099 (9)	−0.0063 (10)
C19	0.0518 (13)	0.0645 (15)	0.0681 (15)	−0.0066 (11)	0.0249 (12)	−0.0020 (12)
C20	0.0731 (16)	0.0662 (15)	0.0538 (14)	−0.0031 (12)	0.0296 (12)	0.0013 (11)
C21	0.0696 (15)	0.0607 (14)	0.0409 (11)	−0.0031 (11)	0.0118 (10)	−0.0010 (10)
C22	0.0507 (11)	0.0418 (11)	0.0426 (10)	−0.0052 (9)	0.0085 (9)	0.0009 (8)
C23	0.292 (10)	0.265 (9)	0.113 (5)	−0.084 (8)	0.052 (5)	0.021 (5)
C24	0.159 (5)	0.199 (6)	0.085 (3)	−0.056 (4)	−0.017 (3)	0.013 (3)
O1	0.0719 (13)	0.1151 (19)	0.0731 (13)	−0.0186 (12)	−0.0158 (10)	0.0113 (13)
Cl1	0.0608 (4)	0.0701 (4)	0.0716 (4)	−0.0080 (3)	0.0074 (3)	0.0155 (3)
Cl2	0.0355 (3)	0.0729 (4)	0.0502 (3)	−0.0067 (2)	0.0067 (2)	−0.0181 (3)
N1	0.0341 (8)	0.0499 (10)	0.0420 (9)	−0.0038 (7)	0.0050 (7)	−0.0029 (7)
N2	0.0366 (8)	0.0493 (10)	0.0392 (8)	−0.0061 (7)	0.0044 (7)	−0.0041 (7)
N3	0.0422 (9)	0.0542 (11)	0.0384 (9)	−0.0065 (7)	0.0015 (7)	−0.0031 (7)

Geometric parameters (Å, °)

Cd1—Cl1	2.4591 (7)	C13—C14	1.367 (4)
Cd1—Cl2	2.5604 (6)	C13—H13	0.9300
Cd1—Cl2^{i}	2.6132 (6)	C14—H14	0.9300
Cd1—N1	2.4636 (16)	C15—N1	1.478 (3)
Cd1—N2	2.2819 (16)	C15—C16	1.491 (3)
C1—C6	1.363 (4)	C15—H15A	0.9700
C1—C2	1.365 (4)	C15—H15B	0.9700
C1—H1	0.9300	C16—N2	1.320 (2)
C2—C3	1.380 (4)	C16—N3	1.343 (2)
C2—H2	0.9300	C17—N2	1.390 (2)
C3—C4	1.376 (3)	C17—C18	1.394 (3)
C3—H3	0.9300	C17—C22	1.400 (3)
C4—C5	1.378 (3)	C18—C19	1.374 (3)
C4—C7	1.518 (3)	C18—H18	0.9300
C5—C6	1.377 (4)	C19—C20	1.387 (3)
C5—H5	0.9300	C19—H19	0.9300
C6—H6	0.9300	C20—C21	1.376 (3)
C7—N1	1.497 (3)	C20—H20	0.9300
C7—H7A	0.9700	C21—C22	1.386 (3)
C7—H7B	0.9700	C21—H21	0.9300
C8—N1	1.491 (3)	C22—N3	1.380 (3)
C8—C9	1.503 (3)	C23—C24	1.483 (7)
C8—H8A	0.9700	C23—H23A	0.9600
C8—H8B	0.9700	C23—H23B	0.9600

C9—C11	1.381 (3)	C23—H23C	0.9600
C9—C10	1.388 (3)	C24—O1	1.422 (5)
C10—C14	1.384 (4)	C24—H24A	0.9700
C10—H10	0.9300	C24—H24B	0.9700
C11—C12	1.381 (4)	O1—H1A	0.8518
C11—H11	0.9300	Cl2—Cd1^{i}	2.6132 (6)
C12—C13	1.374 (4)	N3—H3N	0.8763
C12—H12	0.9300		
N2—Cd1—Cl1	105.92 (5)	C13—C14—H14	120.1
N2—Cd1—N1	73.73 (6)	C10—C14—H14	120.1
Cl1—Cd1—N1	99.07 (4)	N1—C15—C16	110.73 (16)
N2—Cd1—Cl2	96.56 (4)	N1—C15—H15A	109.5
Cl1—Cd1—Cl2	110.19 (2)	C16—C15—H15A	109.5
N1—Cd1—Cl2	150.72 (5)	N1—C15—H15B	109.5
N2—Cd1—Cl2^{i}	148.17 (5)	C16—C15—H15B	109.5
Cl1—Cd1—Cl2^{i}	102.95 (2)	H15A—C15—H15B	108.1
N1—Cd1—Cl2^{i}	88.84 (4)	N2—C16—N3	113.18 (19)
Cl2—Cd1—Cl2^{i}	85.712 (19)	N2—C16—C15	122.84 (18)
C6—C1—C2	119.2 (2)	N3—C16—C15	123.98 (18)
C6—C1—H1	120.4	N2—C17—C18	130.45 (19)
C2—C1—H1	120.4	N2—C17—C22	109.12 (17)
C1—C2—C3	120.7 (3)	C18—C17—C22	120.37 (19)
C1—C2—H2	119.6	C19—C18—C17	117.2 (2)
C3—C2—H2	119.6	C19—C18—H18	121.4
C4—C3—C2	120.7 (3)	C17—C18—H18	121.4
C4—C3—H3	119.6	C18—C19—C20	121.8 (2)
C2—C3—H3	119.6	C18—C19—H19	119.1
C3—C4—C5	117.9 (2)	C20—C19—H19	119.1
C3—C4—C7	121.1 (2)	C21—C20—C19	122.0 (2)
C5—C4—C7	121.0 (2)	C21—C20—H20	119.0
C6—C5—C4	121.1 (2)	C19—C20—H20	119.0
C6—C5—H5	119.4	C20—C21—C22	116.5 (2)
C4—C5—H5	119.4	C20—C21—H21	121.7
C1—C6—C5	120.4 (3)	C22—C21—H21	121.7
C1—C6—H6	119.8	N3—C22—C21	132.5 (2)
C5—C6—H6	119.8	N3—C22—C17	105.40 (17)
N1—C7—C4	115.83 (17)	C21—C22—C17	122.0 (2)
N1—C7—H7A	108.3	C24—C23—H23A	109.5
C4—C7—H7A	108.3	C24—C23—H23B	109.5
N1—C7—H7B	108.3	H23A—C23—H23B	109.5
C4—C7—H7B	108.3	C24—C23—H23C	109.5
H7A—C7—H7B	107.4	H23A—C23—H23C	109.5
N1—C8—C9	113.67 (19)	H23B—C23—H23C	109.5
N1—C8—H8A	108.8	O1—C24—C23	112.2 (4)
C9—C8—H8A	108.8	O1—C24—H24A	109.2
N1—C8—H8B	108.8	C23—C24—H24A	109.2
C9—C8—H8B	108.8	O1—C24—H24B	109.2
H8A—C8—H8B	107.7	C23—C24—H24B	109.2

C11—C9—C10	117.6 (2)	H24A—C24—H24B	107.9
C11—C9—C8	122.1 (2)	C24—O1—H1A	111.3
C10—C9—C8	120.3 (2)	Cd1—Cl2—Cd1^{i}	94.288 (19)
C14—C10—C9	121.1 (2)	C15—N1—C8	113.04 (18)
C14—C10—H10	119.5	C15—N1—C7	109.96 (16)
C9—C10—H10	119.5	C8—N1—C7	110.16 (17)
C12—C11—C9	121.4 (3)	C15—N1—Cd1	103.08 (12)
C12—C11—H11	119.3	C8—N1—Cd1	113.07 (12)
C9—C11—H11	119.3	C7—N1—Cd1	107.19 (12)
C13—C12—C11	119.6 (3)	C16—N2—C17	105.01 (16)
C13—C12—H12	120.2	C16—N2—Cd1	113.20 (13)
C11—C12—H12	120.2	C17—N2—Cd1	140.84 (12)
C14—C13—C12	120.2 (3)	C16—N3—C22	107.20 (16)
C14—C13—H13	119.9	C16—N3—H3N	122.6
C12—C13—H13	119.9	C22—N3—H3N	129.2
C13—C14—C10	119.9 (3)		
C6—C1—C2—C3	0.3 (5)	C16—C15—N1—Cd1	42.3 (2)
C1—C2—C3—C4	0.3 (4)	C9—C8—N1—C15	70.0 (2)
C2—C3—C4—C5	−1.1 (4)	C9—C8—N1—C7	−166.53 (19)
C2—C3—C4—C7	−178.7 (2)	C9—C8—N1—Cd1	−46.6 (2)
C3—C4—C5—C6	1.3 (4)	C4—C7—N1—C15	59.5 (3)
C7—C4—C5—C6	179.0 (2)	C4—C7—N1—C8	−65.7 (2)
C2—C1—C6—C5	−0.1 (4)	C4—C7—N1—Cd1	170.91 (17)
C4—C5—C6—C1	−0.7 (4)	N2—Cd1—N1—C15	−30.53 (12)
C3—C4—C7—N1	−90.2 (3)	Cl1—Cd1—N1—C15	73.52 (13)
C5—C4—C7—N1	92.3 (3)	Cl2—Cd1—N1—C15	−104.44 (14)
N1—C8—C9—C11	−97.0 (3)	Cl2^{i}—Cd1—N1—C15	176.45 (12)
N1—C8—C9—C10	81.7 (3)	N2—Cd1—N1—C8	91.85 (14)
C11—C9—C10—C14	4.5 (4)	Cl1—Cd1—N1—C8	−164.09 (13)
C8—C9—C10—C14	−174.2 (2)	Cl2—Cd1—N1—C8	17.94 (19)
C10—C9—C11—C12	−4.2 (4)	Cl2^{i}—Cd1—N1—C8	−61.17 (14)
C8—C9—C11—C12	174.4 (2)	N2—Cd1—N1—C7	−146.56 (15)
C9—C11—C12—C13	0.5 (4)	Cl1—Cd1—N1—C7	−42.50 (14)
C11—C12—C13—C14	3.0 (4)	Cl2—Cd1—N1—C7	139.53 (12)
C12—C13—C14—C10	−2.7 (4)	Cl2^{i}—Cd1—N1—C7	60.42 (13)
C9—C10—C14—C13	−1.1 (4)	N3—C16—N2—C17	−2.8 (2)
N1—C15—C16—N2	−36.4 (3)	C15—C16—N2—C17	176.9 (2)
N1—C15—C16—N3	143.2 (2)	N3—C16—N2—Cd1	−174.02 (14)
N2—C17—C18—C19	175.3 (2)	C15—C16—N2—Cd1	5.6 (3)
C22—C17—C18—C19	−1.6 (3)	C18—C17—N2—C16	−175.9 (2)
C17—C18—C19—C20	2.0 (4)	C22—C17—N2—C16	1.3 (2)
C18—C19—C20—C21	−1.1 (4)	C18—C17—N2—Cd1	−8.7 (4)
C19—C20—C21—C22	−0.2 (4)	C22—C17—N2—Cd1	168.51 (16)
C20—C21—C22—N3	−176.4 (2)	Cl1—Cd1—N2—C16	−80.52 (14)
C20—C21—C22—C17	0.5 (3)	N1—Cd1—N2—C16	14.50 (14)
N2—C17—C22—N3	0.5 (2)	Cl2—Cd1—N2—C16	166.27 (14)
C18—C17—C22—N3	178.0 (2)	Cl2^{i}—Cd1—N2—C16	73.84 (17)
N2—C17—C22—C21	−177.1 (2)	Cl1—Cd1—N2—C17	112.9 (2)

C18—C17—C22—C21	0.4 (3)	N1—Cd1—N2—C17	−152.0 (2)
N2—Cd1—Cl2—Cd1^{i}	−148.11 (5)	Cl2—Cd1—N2—C17	−0.3 (2)
Cl1—Cd1—Cl2—Cd1^{i}	102.23 (3)	Cl2^{i}—Cd1—N2—C17	−92.7 (2)
N1—Cd1—Cl2—Cd1^{i}	−79.91 (9)	N2—C16—N3—C22	3.2 (2)
Cl2^{i}—Cd1—Cl2—Cd1^{i}	0.0	C15—C16—N3—C22	−176.5 (2)
C16—C15—N1—C8	−80.2 (2)	C21—C22—N3—C16	175.1 (2)
C16—C15—N1—C7	156.29 (18)	C17—C22—N3—C16	−2.1 (2)

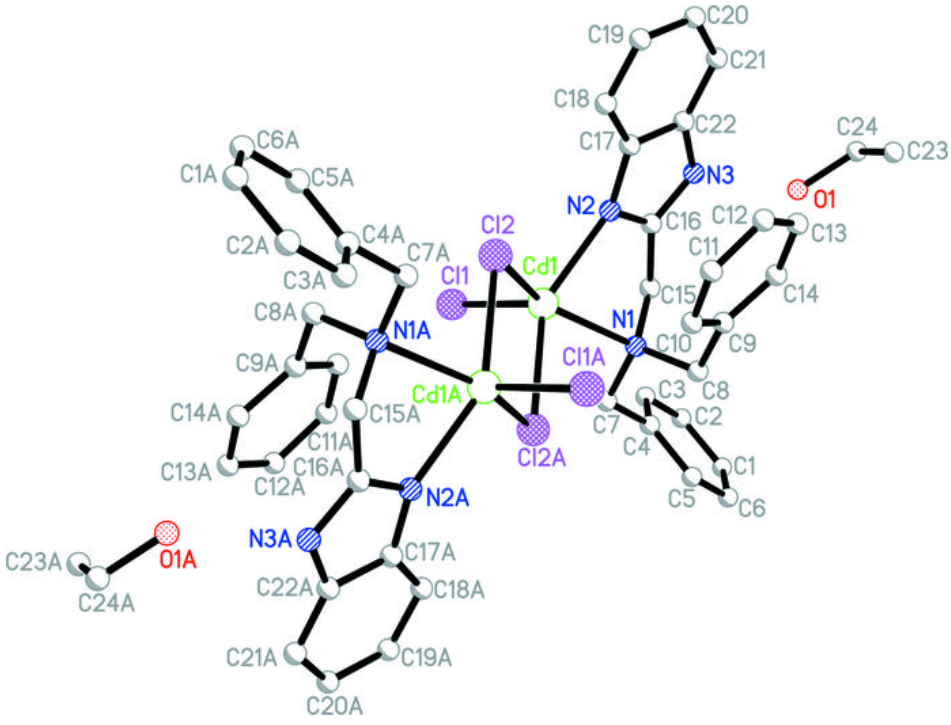
Symmetry codes: (i) −*x*+1, −*y*, −*z*.

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H1A···Cl1^{ii}	0.85	2.33	3.157 (2)	164
N3—H3N···O1	0.88	1.90	2.772 (3)	174

Symmetry codes: (ii) *x*+1/2, −*y*+1/2, *z*+1/2.

Fig. 1


C20
C19
C21
C18
C22
C17
N3
C24
C23
O1
C6A
C1A
C5A
N2
C16
C12
C13
C2A
C4A
C7A
Cl2
Cd1
C11
C3A
Cl1
C15
C14
C8A
N1A
N1
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C11A
C4
C13A
C16A
Cl2A
C1
C12A
N2A
C5
C6
N3A
O1A
C23A
C17A
C24A
C22A
C18A
C21A
C19A
C20A

Fig. 2